MSG No. 126.386 P_I4/nnc [Type IV, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/m'm'm'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[1,2,3,4,5,6,7,8,25,26,27,28,29,30,31,32]
2	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 2: Wyckoff site: `2b`, site symmetry: `4/m'm'm'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[1,2,3,4,5,6,7,8,25,26,27,28,29,30,31,32]
2	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 3: Wyckoff site: `4c`, site symmetry: `m'm'm'.`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[1,4,5,6,25,28,29,30]
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[2,3,7,8,26,27,31,32]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[9,12,13,14,17,20,21,22]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[10,11,15,16,18,19,23,24]

Table 4: Wyckoff site: `4d`, site symmetry: `-4m'2'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,6,10,11,23,24,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[2,3,9,14,20,21,31,32]
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[4,5,15,16,18,19,25,30]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[7,8,12,13,17,22,26,27]

Table 5: Wyckoff site: `4e`, site symmetry: `4m'm'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, z\right]$	[1,2,3,6,28,29,31,32]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}-z\right]$	[4,5,7,8,25,26,27,30]
3	$\left[\frac{1}{4}, \frac{1}{4}, -z\right]$	[9,10,11,14,20,21,23,24]
4	$\left[\frac{1}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	[12,13,15,16,17,18,19,22]

Table 6: Wyckoff site: `8f`, site symmetry: `..2'/m'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,9,24,32]`
2	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[2,10,20,28]`
3	$\left[0,\ \frac{1}{2},\ 0\right]$	`[3,11,21,29]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,12,18,26]`
5	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[5,13,19,27]`
6	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[6,14,23,31]`
7	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[7,15,22,30]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[8,16,17,25]`

Table 7: Wyckoff site: `8g`, site symmetry: `2m'm'.`

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[1,6,28,29]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	`[2,3,31,32]`
3	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[4,5,25,30]`
4	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[7,8,26,27]`
5	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	`[9,14,20,21]`
6	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	`[10,11,23,24]`
7	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[12,13,17,22]`
8	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[15,16,18,19]`

Table 8: Wyckoff site: `8h`, site symmetry: `m'.2m'`

No.	position	mapping
1	$\left[x,\ x,\ \frac{3}{4}\right]$	`[1,7,30,32]`
2	$\left[\frac{1}{2}-x,\ x,\ \frac{3}{4}\right]$	`[2,5,27,28]`
3	$\left[x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[3,4,26,29]`
4	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[6,8,25,31]`
5	$\left[-x,\ -x,\ \frac{1}{4}\right]$	`[9,15,22,24]`
6	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[10,13,19,20]`
7	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[11,12,18,21]`
8	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[14,16,17,23]`

Table 9: Wyckoff site: `8i`, site symmetry: `m'2m'.`

No.	position	mapping
1	$\left[x,\ \frac{3}{4},\ \frac{3}{4}\right]$	`[1,4,29,30]`
2	$\left[\frac{3}{4},\ x,\ \frac{3}{4}\right]$	`[2,7,27,32]`
3	$\left[\frac{3}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[3,8,26,31]`

continued ...

Table 9

No.	position	mapping
4	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	[5,6,25,28]
5	$\left[-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	[9,12,21,22]
6	$\left[\frac{1}{4},\ -x,\ \frac{1}{4}\right]$	[10,15,19,24]
7	$\left[\frac{1}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[11,16,18,23]
8	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{4}\right]$	[13,14,17,20]

Table 10: Wyckoff site: 8j, site symmetry: m'2m'.

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[1,4,29,30]
2	$\left[\frac{1}{4},\ x,\ \frac{3}{4}\right]$	[2,7,27,32]
3	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[3,8,26,31]
4	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[5,6,25,28]
5	$\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[9,12,21,22]
6	$\left[\frac{3}{4},\ -x,\ \frac{1}{4}\right]$	[10,15,19,24]
7	$\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[11,16,18,23]
8	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	[13,14,17,20]

Table 11: Wyckoff site: 16k, site symmetry: ..2'

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	[1,23]
2	$[-x,\ x,\ 0]$	[2,21]
3	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[3,20]
4	$\left[x,\ -x,\ \frac{1}{2}\right]$	[4,19]
5	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[5,18]
6	$\left[\frac{1}{2}-x,\ -x,\ 0\right]$	[6,24]
7	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[7,17]
8	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[8,22]
9	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	[9,31]
10	$[x,\ -x,\ 0]$	[10,29]
11	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ 0\right]$	[11,28]
12	$\left[-x,\ x,\ \frac{1}{2}\right]$	[12,27]
13	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[13,26]
14	$\left[x+\frac{1}{2},\ x,\ 0\right]$	[14,32]
15	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[15,25]
16	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[16,30]

Table 12: Wyckoff site: `16l`, site symmetry: `m'..`

No.	position	mapping
1	$\left[x,\, y,\, \frac{3}{4}\right]$	`[1,30]`
2	$\left[\frac{1}{2}-y,\, x,\, \frac{3}{4}\right]$	`[2,27]`
3	$\left[y,\, \frac{1}{2}-x,\, \frac{3}{4}\right]$	`[3,26]`
4	$\left[x,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	`[4,29]`
5	$\left[\frac{1}{2}-x,\, y,\, \frac{3}{4}\right]$	`[5,28]`
6	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	`[6,25]`
7	$\left[y,\, x,\, \frac{3}{4}\right]$	`[7,32]`
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{3}{4}\right]$	`[8,31]`
9	$\left[-x,\, -y,\, \frac{1}{4}\right]$	`[9,22]`
10	$\left[y+\frac{1}{2},\, -x,\, \frac{1}{4}\right]$	`[10,19]`
11	$\left[-y,\, x+\frac{1}{2},\, \frac{1}{4}\right]$	`[11,18]`
12	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{4}\right]$	`[12,21]`
13	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{4}\right]$	`[13,20]`
14	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	`[14,17]`
15	$\left[-y,\, -x,\, \frac{1}{4}\right]$	`[15,24]`
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{4}\right]$	`[16,23]`

Table 13: Wyckoff site: `16m`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\, x,\, z]$	`[1,32]`
2	$\left[\frac{1}{2}-x,\, x,\, z\right]$	`[2,28]`
3	$\left[x,\, \frac{1}{2}-x,\, z\right]$	`[3,29]`
4	$\left[x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	`[4,26]`
5	$\left[\frac{1}{2}-x,\, x,\, \frac{1}{2}-z\right]$	`[5,27]`
6	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, z\right]$	`[6,31]`
7	$\left[x,\, x,\, \frac{1}{2}-z\right]$	`[7,30]`
8	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	`[8,25]`
9	$[-x,\, -x,\, -z]$	`[9,24]`
10	$\left[x+\frac{1}{2},\, -x,\, -z\right]$	`[10,20]`
11	$\left[-x,\, x+\frac{1}{2},\, -z\right]$	`[11,21]`
12	$\left[-x,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	`[12,18]`
13	$\left[x+\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	`[13,19]`
14	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	`[14,23]`
15	$\left[-x,\, -x,\, z+\frac{1}{2}\right]$	`[15,22]`
16	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	`[16,17]`

Table 14: Wyckoff site: `16n`, site symmetry: `.m'.`

No.	position	mapping
1	$\left[\frac{3}{4},\, y,\, z\right]$	`[1,28]`

continued ...

Table 14

No.	position	mapping
2	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ z\right]$	[2,31]
3	$\left[y,\ \frac{3}{4},\ z\right]$	[3,32]
4	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[4,25]
5	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-z\right]$	[5,30]
6	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ z\right]$	[6,29]
7	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[7,26]
8	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[8,27]
9	$\left[\frac{1}{4},\ -y,\ -z\right]$	[9,20]
10	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[10,23]
11	$\left[-y,\ \frac{1}{4},\ -z\right]$	[11,24]
12	$\left[\frac{1}{4},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[12,17]
13	$\left[\frac{1}{4},\ -y,\ z+\frac{1}{2}\right]$	[13,22]
14	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -z\right]$	[14,21]
15	$\left[-y,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[15,18]
16	$\left[y+\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[16,19]

Table 15: Wyckoff site: 32o, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[2]
3	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[3]
4	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[4]
5	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[5]
6	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[6]
7	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[8]
9	$[-x,\ -y,\ -z]$	[9]
10	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[10]
11	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[11]
12	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[12]
13	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[13]
14	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[14]
15	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[16]
17	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[17]
18	$\left[-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[18]
19	$\left[y+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	[19]
20	$\left[x+\frac{1}{2},\ -y,\ -z\right]$	[20]
21	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[21]
22	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[23]
24	$[-y,\ -x,\ -z]$	[24]
25	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[25]

continued ...

Table 15

No.	position	mapping
26	$\left[y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-y,\ x,\ \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\ y,\ z\right]$	[28]
29	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[29]
30	$\left[x,\ y,\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[31]
32	$[y,\ x,\ z]$	[32]